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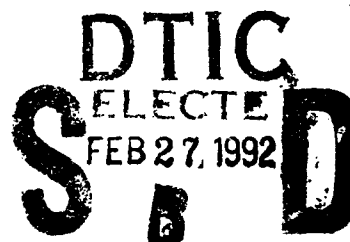
Reflection of X-Rays From Repeated Multilayer Structures

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13. ABSTRACT (Maximum 200 words) A calculation for obtaining the expected reflectivity of soft x-rays from repeated multilayers is described. The calculation is a "classical" or "optical" one in the sense that the incoming radiation is described as a plane wave (rather than a collection of photons), and each layer is assumed to be described by a complex index of refraction (not by discrete atoms). A guide to a computer program incorporating this calculation is provided.				
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CONTENTS

1. INTRODUCTION	1
2. SOFT X-RAY REFLECTION VIA CLASSICAL OPTICS	2
3. INTEGRATED REFLECTIVITY	4
4. SURFACE ROUGHNESS	5
5. DESCRIPTION OF COMPUTER PROGRAM	5
APPENDIX	6
REFERENCES	21



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RELECTION OF X-RAYS FROM REPEATED MULTILAYER STRUCTURES

1. Introduction.

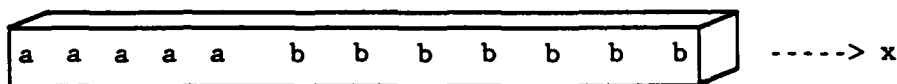
Shortly after x-rays were discovered nearly 100 years ago, it was observed that crystals were able to reflect x-rays, but only in certain directions. The accepted explanation for this phenomenon - called x-ray diffraction - postulates that the crystal consists of simple but infinitely repeated identical "cells" of atoms; for a given wavelength and an arbitrary direction, reflections from the many cells interfere with each other; it is only along a few directions that the reflections from the many repeated cells cooperate (reinforce) to provide a detectable "diffracted" beam. The intensity along each diffracted beam depends on the exact position of each atom in the cell. Two uses, conceptually each other's opposite, result from these facts: on the one hand, crystals can be used to produce desired reflections of x-rays; on the other, observed reflections can be used to determine the detailed atomic structure of the cell. An early, but authoritative, description of these effects appears in ref. [1].

It will be plausible that the phenomenological description and theory summarized above will be appropriate only if the size of the cells and the wavelength of the radiation are of roughly the same size: on the one hand, very short wavelengths "will not notice" the correlation between atoms in a cell, while, on the other, very long ones won't even notice the periodicity. So, if you are interested in reflecting long wavelengths, you might not find natural crystals of large enough cell size; you might have to construct your own. This is the rationale of the attempts, in the last few decades, of constructing repeating "multilayers" as artificial crystals [2]. These are, generally speaking, a thin film of substance A of precisely known thickness (usually, a few atomic layers), followed by a similar layer of substance B; followed by more identical bilayers, ABABABAB....

The diffraction properties of repeating multilayers, usually repeating bilayers, have been studied at the Naval Research Laboratory (NRL) both experimentally and theoretically. For the theoretical work, two approaches have been used:

- 1) an x-ray, or atomistic approach, and
- 2) an electromagnetic, or homogeneous approach.

In 1), a long and thin unit cell is first defined, as shown:



Both a and b atoms are in "ordered", specified positions. This long and thin cell is repeated an infinite number of times in the space directions x, y, and z to form a semi-infinite slab. The reflective properties of the multilayer is then calculated by evaluating the structure factor and other procedures well known to workers in x-ray crystallography; see ref [1]. Corrections are later made for the finiteness of the multilayers, the vibrational motion of the atoms, and the absorptive properties of the layers. The fact that atoms in thin layers are probably in random rather than "ordered" positions is taken as unimportant for long enough wavelengths. For details of this atomistic approach, refer to refs. [3] and [4].

The electromagnetic approach, 2), is the one described in the rest of this report. Each layer is assumed to be homogeneous (non-atomic), the incident radiation is taken to be an electromagnetic wave, and their interaction described by Maxwell's equations. It is thus a purely "classical" (i.e., a non-quantum) theory, containing neither atoms nor photons. At each interface, the electromagnetic wave is split into a refracted and a reflected part given by Fresnel's laws (ref. [4]) (which, of course, are derivable from Maxwell's equations); within the interior of any layer, the wave is attenuated by absorption. We can thus calculate, successively, the properties of the electromagnetic wave after any number of bilayers - until we reach the thickness of the specific multilayer we want to describe, or until absorption has reduced the intensity to a value so low that is no longer interesting.

There is no new physics in this method of calculating the effect of multilayers on electromagnetic radiation (see refs. [5], [6], [7]) . Rather, what is done here is the development of a formalism and a computer program conveniently applicable to a problem of continuing interest at the Naval Research Laboratory [3].

Do the two methods agree? If not, which (if either) is correct, and under what circumstances? We have only partial answers to these very reasonable questions. As noted above, our method 2) is more likely to be valid the longer the wavelength of the radiation; for short waves ("hard x-rays"), atomic interactions cannot be ignored or averaged over and a version of method 1) must be used. On the other hand, method 2) takes more reasonable account of several physical properties: unlike method 1), it does not have to assume strict periodicity on the atomic level; the fact of absorption enters the calculation properly ab initio, rather than as a correction to an absorption-free calculation; and the same is true for the fact that the number of bilayers in the structure under consideration is finite rather than infinite. In addition, method 2) is able to compute the reflectivity at any wavelength and in particular the shape of any reflection line, while method 1) gives only the integrated reflectivity.

2. Soft X-ray Reflection via Classical Optics

a) a single layer

As sketched in figure 1, consider an electromagnetic wave going from region 1 down into regions 2 and region ℓ (mnemonic for future use: ℓ stands for "last"). Born and Wolf (ref [5]; referred to as BW) show that the electromagnetic field at point h_2 is related to that at point 0 by the relation

$$U(h_2) = M_2 \cdot U(0) \quad (1)$$

where $U(h)$ is defined as the 1×2 matrix

$$U(h) = \begin{pmatrix} E(h) \\ H(h) \end{pmatrix} \quad (2)$$

with E and H the electric and magnetic fields, respectively, and M_2 is the 2×2 matrix

$$M_2 = \begin{bmatrix} \cos\beta_2 & -(i/p_2)\sin\beta_2 \\ -(ip_2)\sin\beta_2 & \cos\beta_2 \end{bmatrix} \quad (3a)$$

with

$$\begin{aligned} p_2 &= (n_2/\mu_2) \cos\theta_2 \\ \beta_2 &= (2\pi h_2/\lambda_1) n_2 \cos\theta_2 \\ \sin\theta_2 &= (n_1/n_2) \theta_1 \end{aligned} \quad (3b)$$

Please note that θ is defined as the angle of incidence as measured with respect to the normal to the material surface, as shown in figure 1 and as is customary in literature on optics. (In the field of x-rays, θ usually denotes the

complement of this angle). The subscript 2 in the various quantities indicates that they refer to material "2". The parameters ϵ , μ , n and are the dielectric constant, the magnetic permeability, and the index of refraction; they are related by $\epsilon\mu = n^2$.

We can now use equ. (1) to calculate the field quantities E and H below the layer in terms of their values above it. We think that the reader will find it reasonable that the reflectivity of the layer of material "2" which is h_2 centimeters thick can indeed be calculated from these field quantities. The details - a little lengthy but straightforward - are given by BW in their equs. (48) and (51) of sec. 6.1. The polarization of the incident beam also enters into the calculation.

b) Bilayers and repeated bilayers.

The virtue of the matrix formulation (1) is that the effect of any sequence of layers can now be written down effortlessly: suppose that the layer of material "2" is followed by a layer, h_3 cm thick, of material "3", as shown in figure 2 : then we have

$$U(h_2+h_3) = M_3 \cdot M_2 \cdot U(0) \quad (4)$$

where M_3 is just M_2 with subscripts 2 replaced by 3; and for a sequence of N bilayers of materials 2 and 3 we have simply

$$U[N(h_2+h_3)] = (M_3 \cdot M_2)^N \cdot U(0) \quad (5a)$$

as illustrated in figure 3. To find the reflectivity of these N bilayers, we proceed just as in section 3a) above, except that, in solving (5) instead of (1), we must use the more complicated (but still 2 by 2) product matrix $(M_3 \cdot M_2)^N$ instead of M_2 .

For convenience, rewrite (5a) as

$$U(bottom) = M_{23}^N \cdot U(top) \quad (5b)$$

where

$$M_{23} = M_3 \cdot M_2 \quad (6)$$

is found by direct multiplication, and is written down by BW (their p.67, equ. (86)) and also in our appendix 1. It can be written in the form

$$M_{23} = \begin{pmatrix} a & c \\ d & b \end{pmatrix} \quad (7)$$

Next, we need, for equ.(5), the Nth power of this matrix. We do this by diagonalizing M_{23} ; that is, we find the matrix S which produces

$$S^{-1} M S = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix} \quad (8)$$

(where we have for simplicity dropped the subscripts 23), and also find the "eigenvalues" λ_1 and λ_2 . The eigenvalues of the Nth power of this matrix, needed in (5), come out simply to be λ_1^N and λ_2^N , as is seen from

$$\begin{aligned} S^{-1} M^N S &= S^{-1} M M M \dots M M S \\ &= S^{-1} M (S S^{-1}) M (S S^{-1}) \dots M (S S^{-1}) M S \\ &= (S^{-1} M S) (S^{-1} M S) \dots (S^{-1} M S) \\ &= (S^{-1} M S)^N \end{aligned}$$

which with the use of equ. (8) becomes

$$S^{-1} M^N S = \begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{bmatrix}^N = \begin{bmatrix} \lambda_1^N & 0 \\ 0 & \lambda_2^N \end{bmatrix} \quad (9)$$

or

$$M^N = S^{-1} \begin{bmatrix} \lambda_1^N & 0 \\ 0 & \lambda_2^N \end{bmatrix} S$$

This explains why the number N of multilayers appears in appendix 1 in such a simple way - as an exponent on λ_1 and λ_2 . All we shall need are the explicit values of λ_1 , λ_2 , and S . These come out of the diagonalization process and are given in appendix 2.

We now proceed just as in the last paragraph of section 2a): put (9) into (5b) to get the field quantities E and H below the multiple bilayer from their values above, and calculate the reflectivity from them.

This completes the essentials of the calculation; the details appear in the appendices. Appendix 1 covers the mathematical aspects of this section. Appendix 2 details the diagonalizing transformation of a 2×2 matrix. Appendix 3 shows how the existence of reflection peaks is related to the analytical properties of the eigenvalues of the characteristic matrix. Appendix 4 gives two explicit expressions for the reflectivity r (which was derived in appendix 1), and notes the conditions under which either is preferable for computations. Appendix 5 relates the data for each atomic constituent of a layer to the gross properties (i.e. the index of refraction) of the layer. Appendix 6 reconciles a notational difference between two references. Appendix 7 is a printout of the computer program that is described verbally in section 5.

3. Integrated reflectivity.

The preceding section, together with the details in the appendices, has allowed us to compute the reflectivity of a repeated bilayer at a specified incident wavelength. The obvious next step would seem to be the repetition

of the calculation for a different but nearby angle, until the entire range of theta from 0 to $\pi/2$ has been covered. This is indeed done in our computer program.

A well-known experimental fact in x-ray theory and practice is the existence of "reflection lines"; that is, strong reflection over one (or more) very small regions of wavelength, with (near-)zero reflection between them (see ref.[1]). For a sufficiently large number N of bilayers, our calculations verify this state of affairs. Naturally one then wants to know the "integrated reflectivity" of one line, and this quantity can be obtained by summing (or "numerically integrating") over the wavelengths contained in one line.

We have of course incorporated this into our computer program, but want to warn that inherent arbitrariness remains in the choice of the limits in the integration. The method we have adopted is to put the lower limit of integration 1/3 of the way to the line to the left, and the upper limit 1/3 of the way to the line to the right. This will be fine if each line is indeed "sharp" and if the reflection is very close to 0 in between; but exceptions to this rule will be buried beyond recognition by this choice for limits of integration. Caution is advised.

4. Surface Roughness.

Experimental observation of lines that are broader or weaker than predicted by theory have been plausibly attributed to "surface roughness"; see ref. [5]. Our theoretical model describes layers with two properties:

- 1) boundaries are perfect planes, and
- 2) bilayers are repeated with perfect periodicity.

Neither of these conditions is likely to be fully attained in the real world; it is plausible to attribute the deviations of experimental data from theory to surface roughness.

Can we put surface roughness into our model while maintaining mathematically essential properties 1) and 2)? What we have done is to replace the two layers consisting of pure material A and pure material B by eight layers of the same total thickness; layer 2 is pure A, layer 6 is pure B, and layers 3,4,5 have intermediate index of refraction, as do layers 7,8,9. The procedure is justified in greater detail in ref. [8].

5. Description of Computer program.

A version of the FORTRAN computer program in use, called LA8WC.FOR, is presented in Appendix 7. The line numbers on the far left appear for the reader's convenience only and are ignored by the computer; the set of numbers appearing to the right of the line numbers are FORTRAN statement numbers. The program displayed in Appendix 7 describes a repeated structure of 8 layers, numbered from 2 to 9; layer 2 consists of W (tungsten) and layer 6 of C (carbon); the other layers have an intermediate composition, consisting of tungsten and carbon ions in the ratios 3:1, 1:1, and 1:3. The program can be applied to other multilayer materials by changing a small number of lines between lines 50 and 166.

For easier readability, we always attach a statement number n which ends in 0 to the first statement in each "do loop", and statement number n+1 to the last statement in that loop, e.g. thus:

```
800      do 801 kk=1, 9
```

```
      .  
      .  
      .
```

```
801      continue.
```

The main part of the calculation are the nested lops which start at line number 245:

```
700      sums over the "orders" of the reflection peaks
```

```
200          sums over the two polarizations (TE, TM)
```

```
300              sums over the angles of incidence around a peak
```


400 sums over the layers in one cell

401

301

201

701

The main printout, which is the integrated reflectivity of one peak, is elicited by statement # 50 (at line # 388). However, the (non-integrated) reflectivity at each angle of incidence can also be printed out, by removing the c (= "comment") from statement 66 (at line number 382).

The 244 lines that precede this main calculation will not be described in much detail here, since they are comparatively simple structurally, proceeding in a linear fashion without much nesting or interrelationships. Lines 1 through 33 are explanatory comments; 34 through 49 are FORTRAN declarations of variables. Basically what is done in lines 50 through 166 is the insertion of the data specific to the chemical species involved; they culminate in the calculation of the index of refraction (called n_{ix}) in lines 173- 195, which is the quantity used in the four main loops.

A possible point of confusion- viz. a change in numbering of the layers - is described in lines 205, 206. The reason for this is historical, not logical: this program for the 8 layers per cell was constructed from an earlier one for 4 layers per cell. The program could, of course, be rewritten to give each layer the correct number in the first place.

We have in many cases provided two ways of inserting data, at the option of the operator: from the keyboard, or by modifying a statement in the program. For example, in lines 95-100, densities are inserted by statements in the program. To change to insertion from the keyboard, remove the "!" from line 97, and insert a "!" in lines 98 and 99.

To run the program, the command, to be entered from the "\$" prompt, is

@exnoop la8wc

This calls a short command file, EXNOOP.COM , which provides the usual FORTRAN, link, and run commands without use of the optimizer. The reason for the exclusion of the optimizer is that it often gives wrong answers. This is a problem of the computer we are using that will, we are told, be fixed in the future.

Appendix 1. Mathematical details.

This appendix covers the same ground as sec. 2, but does so in detailed mathematical language, and in notation similar to that used in the computer program (Appendix 7), with minimal verbal explanation.

The results depend on the polarization of the incoming beam. The formulas below refer to TE polarization. TE [= "transverse electric"] means that the Electric field vector E is perpendicular ("Transverse") to the plane of incidence, i.e. to the plane of the paper in figure 1. TM is analogously defined for the Magnetic field H . At the end of this appendix, we explain how the TM formulas can be easily obtained from the TE ones. To describe an unpolarized beam, the TE and TM results should be averaged in the end.

The index i refers to the materials involved. Originally, $i=2$ and 3 referred to the bilayer, which is repeated N times; $i=1$ and l are not repeated; they refer to the materials bounding the repeated bilayers. At the end of this appendix, we explain how the formulas must be modified when the repeated structure consists of more than 2 layers.

Input data are: angle of incidence θ_1 , incident wavelength λ_0 , complex indices of refraction n_i , layer thickness h_2 , h_3 , number of bilayers N (called layno). Note that generally $n_j = (\epsilon_j \mu_j)^{1/2}$, where ϵ and μ are the dielectric constant and the magnetic permeability. We first compute $h = h_2 + h_3$ and then the $\sin \theta_i = (n_1/n_i)$

$\sin \theta_i$. This is Snell's law; note, however, that, as n_i is generally complex, $\sin \theta_i$ is also, contravening the simple interpretation of θ as an "angle". Further:

$$\begin{aligned}
 p_i &= (n_i/\mu_i) \cos \theta_i \\
 \beta_i &= (2\pi/\lambda_0) h_i n_i \cos \theta_i \\
 a &= \cos \beta_2 \cos \beta_3 - (p_3/p_2) \sin \beta_2 \sin \beta_3 \\
 b &= \cos \beta_2 \cos \beta_3 - (p_2/p_3) \sin \beta_2 \sin \beta_3 \\
 c &= -i[(1/p_3) \cos \beta_2 \sin \beta_3 + (1/p_2) \sin \beta_2 \cos \beta_3] \\
 d &= -i[p_3 \cos \beta_2 \sin \beta_3 + p_2 \sin \beta_2 \cos \beta_3] \\
 \Delta &= b-a = [(p_3/p_2) - (p_2/p_3)] \sin \beta_2 \sin \beta_3 \\
 T &= [\Delta^2 + 4cd]^{1/4} \\
 f &= \Delta + T \\
 \lambda_1 &= (1/2) [a + b + T] \\
 \lambda_2 &= (1/2) [a + b - T] \\
 D &= 2 f T \\
 M_{11} &= (4cd\lambda_2^N + f^2 \lambda_2^N)/D \\
 M_{22} &= (4cd\lambda_2^N + f_2 \lambda_1^N)/D \\
 M_{12} &= 2cf (\lambda_1^N - \lambda_2^N)/D \\
 M_{21} &= 2df (\lambda_{1N} - \lambda_2^N)/D \\
 P &= (M_{11} + M_{12} p_t) p_i \\
 Q &= (M_{21} + M_{12}) p_t \\
 r &= (P-Q)/(P+Q) = \text{reflection coefficient} \\
 R &= |r|^2 = \text{reflectivity}
 \end{aligned}$$

The reader of sec. 2 and appendix 2 will recognize the

matrix $\begin{pmatrix} a & c \\ d & b \end{pmatrix}$ as giving the values of E and H below a bilayer in terms of the values above it; the matrix arises from multiplying the characteristic matrices of layer 2 and layer 3. This tells us how to modify the calculations when more than two -- e.g. three -- different layers are present: simply replace equ. (6) by $M_{2N} = M_4 M_3 M_2$, and so on for any number of different layers.

The equations below a, b, c, d extract the reflectivity from the field quantities E and H above and below the N multilayers, as qualitatively explained in sec. 2.

We noted that the above formulas apply to TE polarized radiation. To obtain equivalent results for TM, only one change must be made: for all i, replace $p_i = (n_i/\mu_i) \cos(\theta_i)$ by $p_i = (\mu_i/n_i) \cos(\theta_i)$. See ref. [9].

Appendix 2. Diagonalization of a 2 by 2 matrix.

The process of diagonalizing an n by n matrix is well known, in the sense that is described in many text books (e.g. refs [10], [11]) and carried out in several published computer programs. Numerical methods must generally be used, either from the beginning or, at any rate, before the end. However, the process becomes much simpler for 2 x 2 matrices: the secular equation is then quadratic, and the eigenvalues are thus explicitly obtainable in terms of radicals, as are all other quantities. Hence, everything can be done analytically. Not having found the simple 2 x 2 case described explicitly in the literature, we summarize the results here. We do not derive them, since the reader can easily verify that the S given below does indeed diagonalize M according to equ. (8).

The matrix of interest is given by equ. (6),

$$M = \begin{pmatrix} a & c \\ d & b \end{pmatrix}$$

Its inverse is

$$M^{-1} = \begin{pmatrix} b & -c \\ -d & a \end{pmatrix} / (ab - cd)$$

The eigenvalues defined by equ. (8) are

$$\begin{aligned} \lambda_1 &= (a+b+T)/2 \text{ and} \\ \lambda_2 &= (a+b-T)/2, \text{ where} \\ T &= [a^2 + 4cd]^{1/2} \text{ and} \\ \Delta &= b-a. \end{aligned}$$

The transformation (8) is accomplished by the matrix

$$S = \begin{pmatrix} 2c & -f \\ f & 2d \end{pmatrix}$$

and its inverse is

$$S^{-1} = \begin{pmatrix} 2d & f \\ -f & 2c \end{pmatrix} / (2fT)$$

where

$$f = \Delta + T.$$

Appendix 3. Analytical properties of eigenvalues, and relation to reflectivity peaks.

We begin by writing down the matrix describing one single layer of index n according to equ. (3) of section 2:

$$M = \begin{pmatrix} \cos\gamma & -(i/p)\sin\gamma \\ -(ip)\sin\gamma & \cos\gamma \end{pmatrix} \quad (\text{A3-1})$$

with

$$\begin{aligned} \gamma &= (2\pi h/\lambda_0) \cos\theta_0 \\ p &= (n/\mu) \cos\theta_0 \end{aligned}$$

We note that this is a "unimodular" matrix (which means that its determinant = 1). The matrix describing any number of layers, possibly different ones, is therefore also unimodular, being a product of matrices of the above form; and this is also true for any similarity transform $H M H^{-1}$ of any such product matrix, since the determinant

of H and H^{-1} are each other's reciprocal; in particular it is true for the diagonal matrix whose elements are the eigenvalues λ_1 and λ_2 . That is, the product of the two eigenvalues obeys

$$\lambda_1 \lambda_2 = 1. \quad (\text{A3-2})$$

This relation has a different meaning depending on whether the eigenvalues are real, pure imaginary, or complex.

Real eigenvalues. If one λ is real, then (A3-2) implies that the other is also, and is the first one's reciprocal; and one λ is greater than 1, the other smaller. E.g., if $\lambda = 8$, then $\lambda_2 = 0.125$.

Pure imaginary eigenvalues. Here (A3-2) implies that if one is pure imaginary, the second one is also. If we write $\lambda_1 = iu_1$, $\lambda_2 = iu_2$ (where the u 's are real), then (A3-2) implies that $\lambda_2 = -i/u_1$. E.g. if $\lambda_1 = 10i$, then $\lambda_2 = -i/10$.

Complex eigenvalues. These can be written $\lambda_1 = r_1 \exp(ia)$, $\lambda_2 = r_2 \exp(ib)$ (where a , b , and the r 's are real). To satisfy (A3-2), we must have $b = -a$, so we have

$$\lambda_1 = r_1 \exp(ia), \lambda_2 = r_2 \exp(-ia). \quad (\text{A3-3})$$

Now recall that the trace of a matrix, like the determinant, is invariant under a similarity transformation. We can therefore equate the trace after the transformation to the trace before,

$$\lambda_1 + \lambda_2 = \text{Tr}(M)$$

or, using (A3-3) for the left and (A3-1) for the right,

$$r_1 \exp(ia) + r_2 \exp(-ia) = 2 \cos \gamma. \quad (\text{A3-4})$$

If γ is real, then $\cos \gamma$ is also, and it follows that r_1 and r_2 are equal, since otherwise $\lambda_1 + \lambda_2$ would not be real. So in that case we have

$$\lambda_1 = r \exp(ia) \text{ and } \lambda_2 = r \exp(-ia), \quad (\text{A3-5})$$

i.e. they are each others conjugates.

What is the physical meaning of a real trace? From (A3-1) we see that $\text{Tr}(M)$ is real iff $n = (\epsilon \mu)^{0.5}$ is real, i.e. if there is no absorption in that layer. The matrix M in that case is of the form

$$\begin{bmatrix} \text{real} & \text{imag} \\ \text{imag} & \text{real} \end{bmatrix}.$$

Now multiply that matrix by another of the same structure (Physically: follow that layer with another non-absorbing one). Then the product matrix has the same form also. (This is perhaps not obvious, but easily seen by carrying out the multiplication). That form will, by the same reasoning, persist through any number of multiplications

(physically: through any number of non-absorbing layers). We conclude that the simple relation (A3-5) holds for a multilayer consisting wholly of non-absorbing layers, while in presence of absorption only the more general relation (A3-3) applies.

Now what is the purpose of all this? We want to find the behavior of the multilayer calculation as a function of N , the number of double layers. N appears in the present calculation only in the form λ_1^N and λ_2^N . The limit of large N is particularly important, as is stability: for physical reasons, a constant value should be approached when N gets large.

Neither complex eigenvalues, nor pure imaginary ones, provide that convergence: λ_1^N has the form $\exp(iaN)$, which changes substantially with every unit increase of N ; λ_2^N behaves in the same way. The same is true for pure imaginary eigenvalues. On the other hand, for real eigenvalues, the greater of the two will, when raised to the power N , be much larger than the smaller raised to the same power. The expression for the reflectivity derived in App. 1 contains the eigenvalues in both the numerator and the denominator, and the reflectivity r then becomes independent of both eigenvalues, hence also independent of N ; this is perhaps best seen from eqs. (A4-3). In absence of absorption, that limiting value is 1, the largest possible value. (This requires a short calculation.) In the special case that neither eigenvalue is larger than the other, viz. that they are equal, r vanishes.

We conclude that the large r 's will arise for values of the angle of incidence θ_1 for which the λ 's are real. To find these regions of θ_1 , we wrote a preliminary program called EIGV.FOR, which prints the eigenvalues as a function of θ_1 . This we followed by the final program LAYER.FOR. Together, they verify the above reasoning: large values of r appear only where the eigenvalues are real.

We would also expect that increasing N would increase the reflectivity, and would sharpen the width of the line (i.e. decrease the range of θ_1 for which reflection is substantial). In absence of absorption, the reflectivity approaches 1 as N approaches infinity; if absorption is present, a finite value for the absorption is approached for N large enough to absorb essentially all the incoming radiation, and no further change in the reflectivity should result from increasing N further. We have verified these features by appropriate model calculations.

Appendix 4. Two expressions for the reflectivity suitable for computation.

As the reader can check, the expression for r arrived at in appendix 1 can be written as

$$r = \frac{\lambda_1^N \psi_1 \psi_3 + \lambda_2^N \psi_2 \psi_4}{\lambda_1^N \psi_1 \psi_3 + \lambda_2^N \psi_2 \psi_4} \quad (\text{A4-1})$$

where

$$\begin{aligned} \psi_1 &= 2d + p_1 f \\ \psi_2 &= f - 2p_1 c \\ \psi_{3\pm} &= 2cp_1 \pm f \\ \psi_{4\pm} &= fp_1 \pm 2d \end{aligned} \quad (\text{A4-2})$$

However, in most situations of interest, one of the two terms in the numerator of (A4-1) will be much larger than the other; and the same for the denominator. This follows from two facts derived in appendix 3: high values of

r arise only when the λ 's are real; and the two λ 's are each other's reciprocal. It follows that one λ will be larger than 1 and the other smaller; for the moment, let us call them λ_r and λ_s . If N is a large number (as often it is), λ_r^N will be much larger than λ_s^N , proving the verbal statement following equ. (A4-2). It is therefore a good idea to divide both the numerator and the denominator by λ_r^N . We obtain

$$r = \frac{\psi_{3-} + \lambda_1^{-2N} (\psi_2/\psi_1) \psi_{4+}}{\psi_{3+} + \lambda_1^{-2N} (\psi_2/\psi_1) \psi_{4-}} \quad (\text{A4-3a})$$

suitable when $|\lambda_1| > |\lambda_2|$ and

$$r = \frac{\psi_{4+} + \lambda_2^{-2N} (\psi_1/\psi_2) \psi_{3-}}{\psi_{4-} + \lambda_2^{-2N} (\psi_1/\psi_2) \psi_{3+}} \quad (\text{4-3b})$$

suitable when $|\lambda_2| > |\lambda_1|$. Note that both (A4-3a) and (A4-3b) are exact in all cases; but in most cases only one of them will allow the computer to proceed without complaining about "overflow" and "underflow".

Appendix 5. Index of refraction n and atomic scattering factor f .

Our calculation requires the index of refraction for each of the atomic species involved and at the incident wavelength of interest. We use the relationship given by James, ref [12]:

$$n = 1 - \delta = 1 - (N\lambda^2 e^2 / 2\pi mc^2) f(0) \quad (\text{A5-1})$$

Here N is the number of atoms per unit volume, λ the incident wavelength, e and m the charge and mass of the electron, and c the speed of light; f is the atomic scattering factor, and the argument (0) denotes grazing incidence.

f can be obtained in two ways. The preferred way uses the tables of Henke et al., ref. [13], where two quantities, f_1 and f_2 , are tabulated for 94 atomic species and many wavelengths. They are the real and imaginary parts of $f(0)$. That is,

$$f(0) = f_1 + i f_2$$

where

$$f_1 = Z + f'$$

and

$$f_2 = f''$$

Z is the atomic number, and $f' + if''$ is commonly called the "anomalous scattering factor".

For wavelengths not covered by Henke, the scattering factors are taken from Cromer [14], who gives f' and f'' in his equs (8) and (9). However, a numerical integration is required to evaluate equ (7) (in contrast to Henke's data, which only need to be looked up).

As a practical matter, a user-friendly computer program due to D.B. Brown, called XTALR.COM exists, ref. [3], which in its preliminary stages finds f in just the manner described above - i.e. by using Henke's numbers when available, and computing them according to Cromer when not. Considerable time may be saved by utilizing that program.

Finally, a word about the index of refraction of a layer containing several different atomic species. Since each atom contributes additively, relation (A5-1) can be used with two modifications: substitute $\sum f_i(0)$ for $f(0)$, where the index i sums over all the atoms in a "cell"; and reinterpret N as the number of "cells" per unit volume.

Appendix 6. Sign change for f'' .

Our analysis (Sec.2) is based on BW, ref. [4], but we also use formulas from J , ref. [12], and data from H, ref. [13]. We must therefore make sure that the notation in these three papers is consistent; or to make appropriate changes where it is not.

We have found one inconsistency: BW and H write

$$\text{Re}[\exp(+inkx)]$$

for a plane wave, while J writes

$$\text{Re}[\exp(-inkx)].$$

Since J is the one who is out of step, the easiest way to make our calculation consistent is to modify J's formulas whenever they are used: we must replace his $\text{Im}(n)$ by $-\text{Im}(n)$. A detailed validation of this procedure is given in ref. [15].

Appendix 7. Printout of computer program.

We present here a printout of a computer program called LA8WC.FOR. The many comments should help its readability; however, the summary in sec. 5 of this report should prove more coherent.

```

1      c      Program LA8WC.FOR
2      c      H. B. Rosenstock, 1990-1991
3
4
5
6
7
8
9      c      program with eight layers- W, C, and 6 mixed ones
10     c      cgs units unless otherwise stated.
11     c      General notation according to Born and Wolf.
12     c      mu, eps, ninx = mag. permeability, diel. constant, index of refr.
13     c      theta(i) are angles of beam with the normal (not with the plane!) in material i.
14     c      the1(1000) are 1000 values of theta(1) above
15     c      h(2), h(3) are thickness of materials 2 and 3,
16     c      wavelength0, k0= wavelength, wave-number
17     c      ha, wavelengthang0, kang0 = same in Angstroms
18     c      subno= # of components(single layers) in one multilayer
19     c      (not counting vacuum at both ends)
20     c      layno= N= # of multilayers; Ndens= # of atoms/vol; Navo= Avogadro's no.;
21     c      Zat,Aat= at. charge,mass; Zat is not used in the calculation
22     c      proper, but may be needed to call the Henke tables.
23     c      ii= sqrt(-1)
24     c      300-301 theta-loop
25     c      400-401 materials loop (inside theta-loop)
26     c      350-310 - see BW sec. 6.1, HBR notes, also,p(4), beta(4)

```

```

27 c      500-loop provides printout for 300 loop, printing maxima and
28 c      minima of reflectivity only.
29
30
31
32
33      implicit real(a-z)
34      complex ii, c, d, discr, f, lam1, lam2
35      complex refl
36      complex ninx, sinthe, costhe, beta, p, theta, decre
37      complex cb2, cb3, sb2, sb3, p2, p3, a, b, delta
38      complex psi1, psi2, psi3pl, psi3mi, psi4pl, psi4mi
39      complex termpl, termmi, top, bot, fstar, fsum, tran, prod
40      parameter(max=26)
41      dimension mu(max), ninx(max), Asum(max), fsum(max)
42      dimension h(max), ha(max)
43      dimension theta(max), sinthe(max), costhe(max), rho(max)
44      dimension Aat(max,10), Zat(max,10)
45      dimension multy(max,10), Ndens(max), p(max), beta(max)
46      dimension f1(max,10), f2(max,10), fstar(max,10), th1peak(0:10)
47      dimension th1diff(0:10)
48      dimension tran(2:max, 2,2), prod(2:max, 2,2)
49
50      ii = (0,1)
51      pi = 3.1415926
52      Navo = 6.02e23 !Avogadro
53      eel = 4.803e-10 !el. charge
54      mel = 9.109e-28 !el. mass
55      clight = 3.00e10 !speed
56
57      0      type 1
58      1      format (' write a label')
59      accept*
60      c      layno = 1
61      3      print 4
62      4      format (' type the number of distinct layers; and
63      2      of multilayers ')
64      ! accept*, subno, layno
65      subno = 8
66      layno = 600
67      10     print 11, subno, layno
68      11     format (' number layers in one multilayer;
69      2      and of multilayers N =', 2f6.0 )
70      type 2
71      dim = 26 !not to exceed stated dimensionality of ninx,mu, etc
72      120    do 121 i = 1, dim      ! initial settings; change them later
73              ninx(i) = 1 ! i sums over the 9 layers (1,9= vacuum)
74              mu(i) = 1
75              ha(i) = 0
76      130    do 131 kk = 1, 9      ! kk sums over atoms in layer i
77              f1(i,kk) = 0
78              f2(i,kk) = 0

```



```

79             Aat(i,kk)= 0
80             Zat(i,kk)= 0
81             multy(i,kk)= 0
82 131         continue
83 121         continue
84 5           type 6
85 6           format( ' type atomic numbers Zat(2,1), (4,1),(4,2); then
86 2 same for atomic masses Aat ')
87 !          accept*, Zat(2), Zat(4), Aat(2), Aat(4)
88             Zat(2,1)= 74
89             Zat(4,1)= 6
90 !          Zat(4,2)= 7
91             Aat(2,1)= 183.9
92             Aat(4,1)= 12.01
93 !          Aat(4,2)= 14.01
94             type*, Zat(2,1),Zat(4,1),Zat(4,2),Aat(2,1),Aat(4,1),Aat(4,2)
95 7           type 8
96             format( ' type densities rho(2) and rho(4) in grams/cc')
97 !          accept*, rho(2), rho(4)
98             rho(2)= 19.3
99             rho(4)= 2.00
100            type*, rho(2), rho(4)
101            print 2
102
103            type 2
104 37          type 38
105 38          format (' for layer 2, type f1, and f2 ')
106            ! accept*, f1(2,1), f2(2,1)
107            f1(2,1)= 43.25
108            f2(2,1)= 11.54
109            type*, f1(2,1), f2(2,1)
110 47          type 48
111 48          format (' for layer 3, type the f1s, and the f2s ')
112            ! accept*, f1(4,1) f2(4,1), f1(4,2), f2(4,2)
113            f1(4,1)= 6.24
114            f2(4,1)= .305
115            f1(4,2)= 0.0 !7.12
116            f2(4,2)= 0.0 !1.96
117            type*, f1(4,1), f2(4,1), f1(4,2), f2(4,2)
118
119            type 2
120            multy(2,1)= 1
121            multy(4,1)= 1
122            multy(4,2)= 0
123 27          type 28, multy(2,1), multy(4,1), multy(4,2)
124 28          format(' multiplicities', 3f5.0 )
125            type 2
126 2           format (' ')
127
128 21          type 22
129 22          format(' type incident wavelength in Angstroms')
130            ! accept*, wavelengthang0

```

```

131      wavelengthang0= 8.34
132      kang0= 2*pi/wavelengthang0
133      wavelength0= wavelengthang0* 1e-8
134      k0= kang0* 1e8
135  30    type 31 , wavelengthang0, kang0
136  31    format (' wavelengthang0, kang0 =' 2f6.2, ' Angstroms, ^-1')
137      print 2
138      ! ha(3)= 0.00
139      ! ha(5)= ha(3)
140      ! ha(2)= 7.672 - ha(3)
141      ! ha(4)= 19.728 - ha(3)
142      ! ha(6)= ha(2)
143      ! ha(7)= ha(3)
144      ! ha(8)= ha(4)
145      ! ha(9)= ha(5)
146
147      ha345= 3.          ! total thickness of layers 3 + 4 + 5
148      ha(2)= 7.672 - ha345
149      ha(6)= 19.728 - ha345
150      ha(3)= ha345/ 3.
151      ha(4)= ha345/ 3.
152      ha(5)= ha345/ 3.
153      ha(7)= ha345/ 3.
154      ha(8)= ha345/ 3.
155      ha(9)= ha345/ 3.
156  160    type 161, ha345
157  161    format (' total thickness of three mixed layers is',f5.2 )
158
159      hsum= 0
160  110    do 111 i=1,dim
161      !      type*, i, ha(i)
162              h(i)= ha(i)* 1e-8
163              hsum= hsum+ h(i)
164      !      type*, hsum
165  111    continue
166      hh= hsum
167  150    type 151
168  151    format (' pause, then enter')
169      accept*
170
171  40     print 41
172  41     format (' i      mu          n          ha')
173  100    do 101 i= 2, subno+1
174      !      compute index of refr. acc. to R.W.James, equ.(2.61)
175      etanum= wavelength0**2* eel**2* Navo
176      etaden= 2* pi* mel* clight**2
177      eta= etanum/ etaden
178      Asum(i)= 0
179      fsum(i)= 0
180      decre= 0
181  800    do 801 kk=1,9
182              fstar(i,kk)= f1(i,kk)- ii* f2(i,kk)

```

```

183          ! see HBR 11Jul89.rep for source of minus-sign above
184          fsum(i)= fsum(i)+ multy(i,kk)* fstar(i,kk)
185          Asum(i)= Asum(i)+ multy(i,kk)* Aat(i,kk)
186      801      continue
187      !      next three lines for "vacant" layer (all Aat zero)
188      805      if (Asum(i) .gt. .1) goto 806
189          ! set ninx(3) and (5) equal to 1
190          decre= 0
191          goto 807
192      806      decre= eta* rho(i)* fsum(i)/ Asum(i)
193      807      ninx(i)= 1- decre
194
195      101      continue
196      type 2
197      ! change ninx(3) and (5) equal to average of the thick ones
198      !      ninx(3)= ( ninx(2)+ninx(4) )/ 2
199      !      ninx(5)= ( ninx(2)+ninx(4) )/ 2
200      ! ninx(6)= ninx(2)
201      ! ninx(7)= ninx(3)
202      ! ninx(8)= ninx(4)
203      ! ninx(9)= ninx(5)
204
205      ! above, ninx(2) describes W, and ninx(4) describes C
206      ! below, ninx(2) describes W, and ninx(6) describes C
207
208      ninx(6)= ninx(4)          ! the C layer
209      ninx(3)= .75* ninx(2)+ .25* ninx(6)
210      ninx(4)= .50* ninx(2)+ .50* ninx(6)
211      ninx(5)= .25* ninx(2)+ .75* ninx(6)
212      ninx(7)= ninx(5)
213      ninx(8)= ninx(4)
214      ninx(9)= ninx(3)
215
216      1100      do 1101 i=2, subno+1
217          ! print the new values for all i
218          type 103, i, mu(i), ninx(i), ha(i)
219      103      format( f4.0, f10.6, ' ', 2f10.6, f12.6)
220      1101      continue
221      print 2
222
223
224      c      locate reflection peaks from Bragg's law; and the distance
225      c      between adjacent ones
226      thlpeak(0)= pi/2
227      omax= 8 ! number of "orders" we consider
228      600      do 601 m6=1, omax
229          right= m6* wavelength0/ (2* hh)
230          !      type*, m6, hh, right
231          if (right .gt. 1) goto 602
232          thlpeak(m6)= acos(right)
233          thldiff(m6)= -thlpeak(m6)+ thlpeak(m6-1)
234      620      type 621, int(m6+.01), thlpeak(m6)

```

```

235 621          format(' peak', i4, ' at', f8.4, ' radians' )
236 601  continue
237 602  continue
238      m6max= m6- 1
239      th1diff(m6max+1)= th1peak(m6max)
240      type 2
241
242  c      the main nested loops follow now. 700 loop sums over the
243  c      reflection peaks (the "orders"); 200 loop sums over pol's
244  c      (TE or TM ); 300 loop over incident angles around the peak.
245 700  do 701 m7= 1, m6max
246      type 2
247 710      type 711
248 711      format (' pause, then enter')
249      accept*
250 720      type 721, int(m7+.01), th1peak(m7)
251 721      format(' peak', i2, ' at', f8.4, ' radians' )
252  c      The "integrated reflectivity" is found by summing the
253  c      reflectivity from thmin to thmax, each of which are located 1/3
254  c      of the way to the next peak
255      thcent= th1peak(m7)
256      thmin= thcent- th1diff(m7+1)/3
257      thmax= thcent+ th1diff(m7 )/3
258      thstep= .001
259 44      type 45, thmin, thcent, thmax, thstep
260 45      format (' min, center, max, step of theta =', 4f8.4)
261      print 2
262
263 200  do 201 pol= 1, 2
264 205  if (pol .lt. 1.5) goto 206
265      type 207
266 207      format (' TM polarization' )
267      goto 208
268 206      continue
269      type 209
270 209      format (' TE polarization' )
271 208  continue
272 42      type 43
273 43      format (' theta1 abs{refl} [col2]**2')
274      j= -1
275      sum=0
276 300  do 301 theta1= thmin, thmax, thstep
277      j= j+1
278      theta(1)= theta1
279 400  do 401 i=1, dim
280      sinthe(i)= ( ninx(1)/ninx(i) ) * sin(theta(1))
281      if ( Real(sinthe(i)) .gt. 1 ) goto 9000
282      ! compute costhe from sinthe;
283      costhe(i)= ( 1- sinthe(i)**2 ) **(.5)
284      p(i)= costhe(i)* ninx(i)/ mu(i)
285      ! TE or TM polarization
286 220  if (pol .lt. 1.5) goto 221

```

```

287          p(i)= costhe(i)* mu(i)/ ninx(i)
288      221      continue
289          beta(i)= costhe(i)* ninx(i)* h(i)* k0
290      401      continue
291          p1= p(1)
292          plast= p(subno+2)
293          !plast is the p for the last layer
294          cb2= cos(beta(2))
295          cb3= cos(beta(3))
296          sb2= sin(beta(2))
297          sb3= sin(beta(3))
298          ! insert the new calculation of lam1 and lam2 here
299          jjmax=subno+ 1
300      84      do 85 jj= 2, jjmax
301          ! define the transfer matrix for layer jj
302          tran(jj, 1,1)= cos(beta(jj))
303          tran(jj, 2,2)= cos(beta(jj))
304          tran(jj, 1,2)= -ii* sin(beta(jj))/ p(jj)
305          tran(jj, 2,1)= -ii* sin(beta(jj))* p(jj)
306      184          !print 185, jj
307      185          !format(' tran[' , f3.0, ']' )
308      284          !type 285, tran(jj,1,1), tran(jj,1,2)
309          !type 285, tran(jj,2,1), tran(jj,2,2)
310      285          !format (2e12.2, ' ', ,2e12.2)
311          !type 2
312      85      continue
313          ! type 2

314      ! the product matrix for the 1st layer (layer 2)
315      prod(2, 1,1)= tran(2, 1,1)
316      prod(2, 1,2)= tran(2, 1,2)
317      prod(2, 2,1)= tran(2, 2,1)
318      prod(2, 2,2)= tran(2, 2,2)
319      87      do 88 jj= 3, jjmax
320          ! the product matrices for the other layers
321          prod(jj,1,1)= prod(jj-1,1,1)* tran(jj,1,1) +
322      2          prod(jj-1,1,2)* tran(jj,2,1)
323          prod(jj,1,2)= prod(jj-1,1,1)* tran(jj,1,2) +
324      2          prod(jj-1,1,2)* tran(jj,2,2)
325          prod(jj,2,1)= prod(jj-1,2,1)* tran(jj,1,1) +
326      2          prod(jj-1,2,2)* tran(jj,2,1)
327          prod(jj,2,2)= prod(jj-1,2,1)* tran(jj,1,2) +
328      2          prod(jj-1,2,2)* tran(jj,2,2)
329      !384          print 385, jj
330      !385          format(' prod[' , f3.0, ']' )
331      !484          type 485, prod(jj,1,1), prod(jj,1,2)
332      !          type 285, prod(jj,2,1), prod(jj,2,2)
333      !485          format (2e12.2, ' ', ,2e12.2)
334      !          type 2

```

```

335      88      continue
336                      !stop
337      a= prod(ijmax, 1,1)
338      b= prod(ijmax, 2,2)
339      c= prod(ijmax, 1,2)
340      d= prod(ijmax, 2,1)
341
342      delta= b-a
343      discr= ( delta**2 + 4*c*d )**.5
344      f= delta+ discr
345      lam1= (a+b+discr)/ 2
346      lam2= (a+b-discr)/ 2
347      abslam1= abs(lam1)
348      abslam2= abs(lam2)
349      !          type*, lam1, lam2, lam1*lam2
350      !          type 2
351      c          now follow two evaluations of refl.
352      c          490 determines which is used; the other,
353      c          though also exact, might lead to overflow.
354      psi1= 2*d+ plast*f
355      psi2= f- 2*plast*c
356      psi3pl= 2*c*p1+ f
357      psi3mi= 2*c*p1- f
358      psi4pl= f*p1+ 2*d
359      psi4mi= f*p1- 2*d
360
361      490      if ( abslam1 .lt. abslam2) goto 491
362                  termpl= psi2* psi4pl/ psi1
363                  termmi= psi2* psi4mi/ psi1
364                  top= psi3mi+ termpl*lam2**(2*layno)
365                  bot= psi3pl+ termmi*lam2**(2*layno)
366                  refl= top/ bot
367                  goto 351
368      491      continue
369                  termpl= psi1* psi3pl/ psi2
370                  termmi= psi1* psi3mi/ psi2
371                  top= psi4pl+ termmi*lam1**(2*layno)
372                  bot= psi4mi+ termpl*lam1**(2*layno)
373                  refl= top/ bot
374
375      351      continue
376      c      no longer needed          avrefl(j)= abs(refl)
377      rr= abs(refl)**2
378          ! print only values above "floor"
379          floor= .0
380      70          if (abs(refl) .lt. floor) goto 71
381      c          if (mod(j,10.) .gt . 0) goto 71
382      c          preceding line cuts down on the printout
383      c66      print 67, theta1, abs(refl), rr
384      67      format (2f8.4, f9.5)
385      71      continue
386      sum= sum+ rr

```

```

387 301 continue
388      rrinteg= thstep* sum
389 50 type 51, rrinteg
390 51 format(' integrated reflectivity= ', e12.3 )
391 302 goto 303
392 9000 type 9001, theta1
393 9001 format (' no penetration for theta1 greater than', f8.4)
394 303 type 2
395 201 continue
396 701 continue
397 !90 type 91, floor
398 91 format (' floor= ', f3.2)
399
400 9999 end
401
402
403

```

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- [6] P.H. Berning, Physics of Thin Films **1**, 69 (1963).
- [7] W.R. Hunter, personal communication.
- [8] D.B. Brown, H.B. Rosenstock, internal reports EM A 25, EM A 26, (unpublished).
- [9] The sentence containing containing equ. (52) on page 60 of BW may be misleading. All π need to be replaced by the corresponding q , not just p_1 and p_1 . See eqs. (38) and (40) on page 58 to verify this.
- [10] H. Margenau & G.M. Murphy," The Mathematics of Physics and Chemistry, "(VanNostrand, New York, 1943), p.304-5.
- [11] L.I. Schiff, "Quantum Mechanics" (3rd edition, McGraw-Hill, New York,1955) p.125-6.
- [12] R.W. James, "The Optical Principles of the Diffraction of X-rays" (1958, G.Bell and sons, London), page 54, equ. (2.61) and below.
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- [15] H.B.Rosenstock, internal report EM A 12 (11Jul90.rep), unpublished.

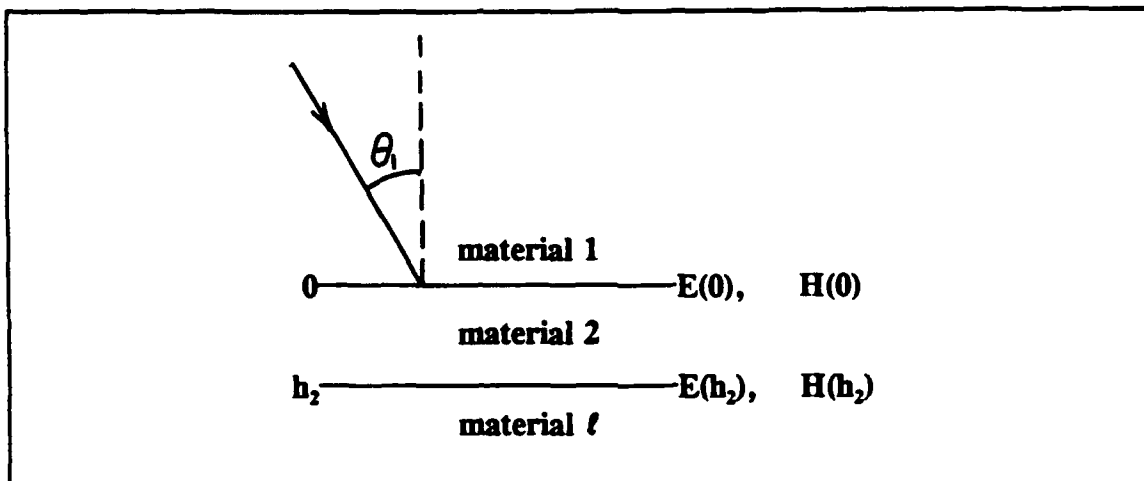


Figure 1. Beam entering a single layer

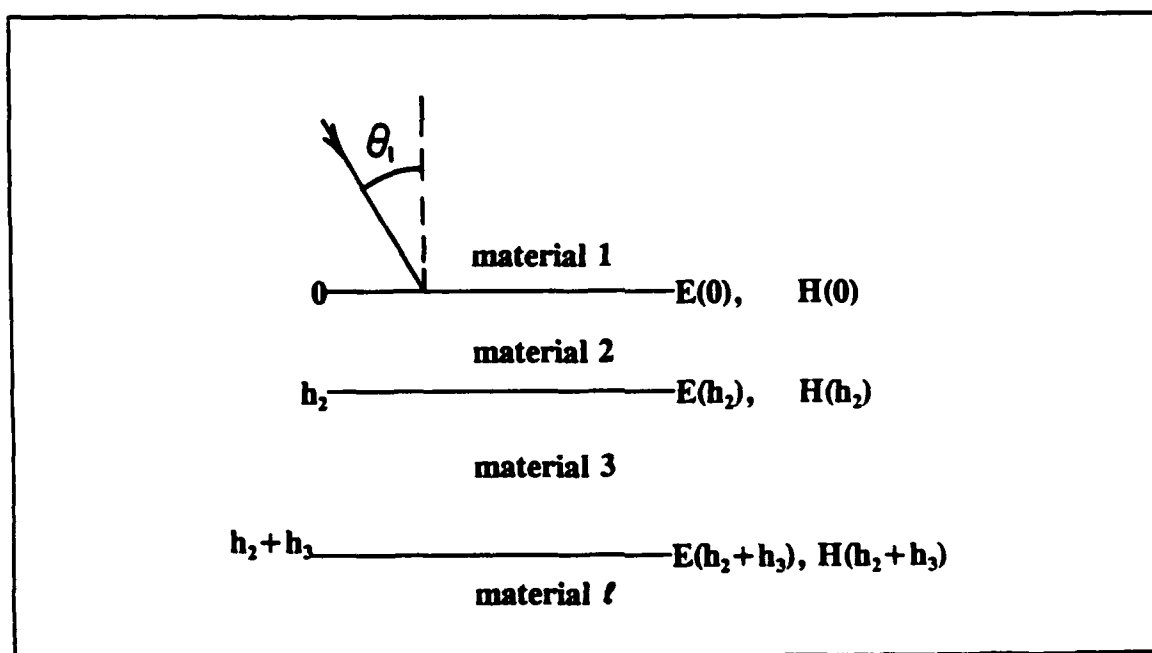


Figure 2. Beam entering a double layer.

